Erratum: Development of Electron-Proton Density Functionals for Multicomponent Density Functional Theory [Phys. Rev. Lett. 101, 153001 (2008)]

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A typographical error in Eq. (9) has been discovered. The first term on the right-hand side of this equation is missing a minus sign. The correct version of Eq. (9) is

$$E_{epc}[\rho^e, \rho^p] = -\iint d\mathbf{r}_1^e d\mathbf{r}_1^p \rho^{ep}(\mathbf{r}_1^e, \mathbf{r}_1^p)/|\mathbf{r}_1^e - \mathbf{r}_1^p| - J_{ep}[\rho^e, \rho^p].$$

This error was simply typographical and was correct in the code. In addition, we identified problems in the input files and the code. The corrected values in Table I are provided here. For all calculations, the He-He distance was fixed to 2.25 Å. These changes do not impact the conclusions of the Letter. Current research is aimed at increasing the electronic and nuclear basis sets and refining the geminal parameters to improve the accuracy of the calculations.

We are grateful to Dr. Chet Swalina in our research group for assistance in the identification and resolution of these errors.

TABLE I. The frequencies in cm^{-1} for the $[He\text{-}H\text{-}He]^+$ system with H, D, and T. The frequencies were determined from a Gaussian fit of the nuclear density along the He-He axis.

	NEO-HF[a,b]	NEO-XCHF[a,b]	FGH[a,b]	NEO-DFT[b,c]	ΔE[d]
H	2506	1432	1183	1279	−0.0115
D	1776	1066	804	805	−0.0090
T	1495	853	641	604	−0.0077

[a]Results from A. Chakraborty, M. V. Pak, and S. Hammes-Schiffer, J. Chem. Phys. **134**, 079902 (2011). NEO-HF is Eq. (10) with $g = 0$.

[b]All calculations used an STO-2G electronic basis set. NEO calculations used the 5s nuclear basis sets for H, D, and T.

[c]The electron-proton functional used a single geminal function with $b = 0.852$ a.u. and $\gamma = 1.962$ a.u. These parameters were fixed at their original values.

[d]$\Delta E = E_{\text{NEO-DFT}} - E_{\text{NEO-HF}}$ is the difference in total energies in a.u.

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